HRAM Selectivity with Confidence

For Routine Applications

Proven • Durable • Affordable

Thermo
SCIENTIFIC

Transforming Routine Quantitation

Designed for routine applications, the Thermo Scientific™ Q Exactive™ Focus hybrid quadrupole-Orbitrap mass spectrometer democratizes high resolution accurate mass (HRAM) analysis, enabling highly selective quantitative and qualitative analysis in a single affordable system.

Built on the proven performance of the Q Exactive platform, the Q Exactive Focus mass spectrometer utilizes the same quadrupole design and Orbitrap™ technology for stable system operation and exceptional analytical performance, enabling labs performing routine analysis in a wide range of applications.

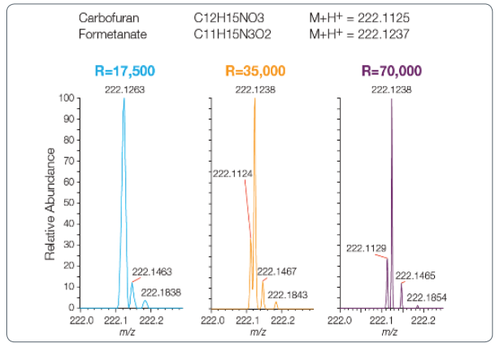
- RF Lens ion source provides the enhanced sensitivity needed to find more analytes in your samples
- Hyperbolic quadrupole mass filter enables precise precursor ion selection and outstanding transmission for more accurate quantitation of low-abundance analytes in complex matrices
- Orbitrap mass analyzer provides a resolution up to 70,000 at *m/z* 200 and mass accuracy of less than 1 ppm enabling high confidence identification of small molecule compounds
- Variable Data-Independent Acquisition (vDIA) delivers reproducible quantitation with complete qualitative confidence for unknown screening
- High speed scan-to-scan polarity switching in both MS and MS/MS modes reveals more compounds in a single run, increasing analytical productivity

Redefining routine analyses

The Q Exactive Focus mass spectrometer brings the benefits of HRAM data, plus proven system reliability, to laboratories performing routine analyses ranging from targeted quantification to non-targeted screening. HRAM MS allows you to detect and quantify all precursor ions in a sample without the need for individual compound tuning and optimization as required with triple quadrupole based quantitation. The Q Exactive Focus MS system enables highly selective detection and quantitation of both targeted and non-targeted compounds in complex matrices with minimal method development, saving time and increasing lab productivity.

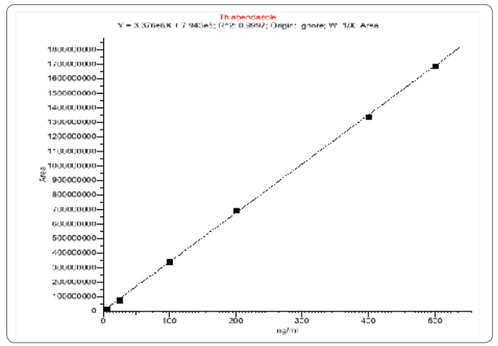
Confident identification enabled by Orbitrap high resolution

The 70,000 resolution and 1 ppm mass accuracy performance of the Q Exactive Focus MS redefines the standard for accurate quantitation and identification by effectively resolving analytes from interferences in highly complex matrices.



Up to 6 orders of magnitude of linear dynamic range covers a wide range of concentrations

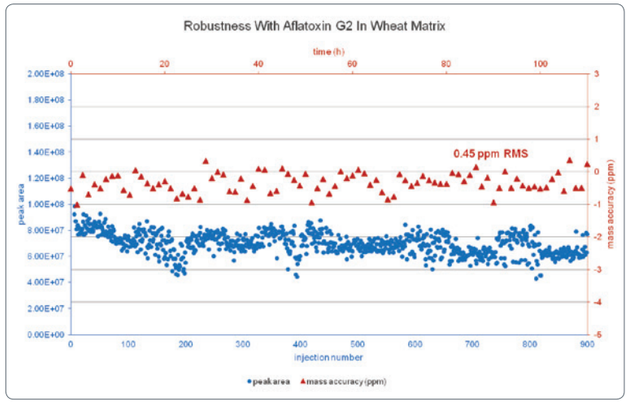
The Q Exactive Focus MS offers quantitative analyses at up to 6 orders of magnitude of linear quantitative dynamic range.



HRAM MS/MS for analytical confidence

The Q Exactive Focus system can perform data-dependent "top 2 MS/MS" to generate spectra confirming analyte identification. A new acquisition mode, Variable Data Independent Analysis (vDIA), wherein all precursor ions are fragmented, creates a digital data archive for detection and potential retrospective quantification of all compounds in a sample.

Robustness of Q Exactive Focus MS: Peak intensity variation during 900 injections (blue) of wheat matrix, showing peak area and mass accuracy stability (peak apex scan, aflatoxin G2, red).



Durability

The proven ruggedness and reliability of the high resolution accurate mass Orbitrap detection delivers the qualitative and quantitative results in a single system, all day, every day.

Environmental and Food Safety

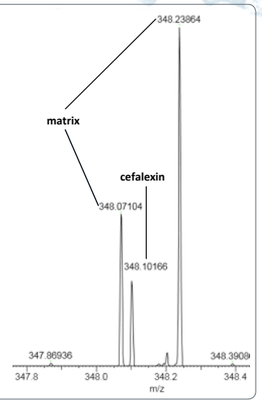
Food and environmental safety testing require analysis of large lists of target compounds to help identify food fraud, and/or food and environmental contamination. With heightened safety concerns, it is increasingly important to screen growing lists of compounds which may be present. Built-in methods and databases for non-targeted compound analysis enable the identification and quantitation of samples more effectively and faster, expanding a lab's monitoring capabilities. Combined with Thermo Scientific™ TraceFinder™ software, the Q Exactive Focus MS offers a powerful, yet simple to use, solution for routine analysis laboratories with the durability demanded by routine analysis laboratories.

HRAM Quantitation built on proven Orbitrap technology

Quantitative tasks can be run without compromise, delivering high sensitivity, accurate quantitation and excellent linear dynamic range. Automated data processing with TraceFinder software makes routine analyses quick and easy. With full scan HRAM quantitation, no sample specific method optimization is necessary, and the risk of missing important non-targeted compounds is greatly reduced.

Sensitivity levels for a representative sample set of veterinary drugs.

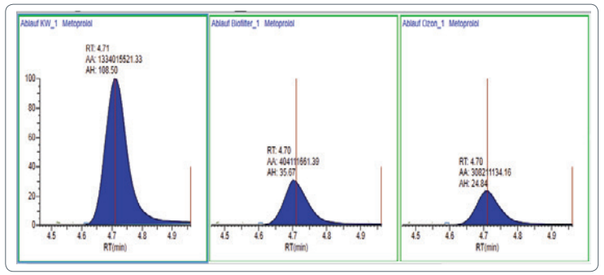
Compound	FS-ddMS2 [ppb]	Compound	FS-ddMS2 [ppb]
Abamectin*	50.0	Marbofloxacine	0.5
Amoxicillin	1.0	Metronidazole	0.1
Ampicillin	0.5	Metronidazole-OH	0.5
Cefalexin	0.5	Moxidectin	0.5
Cefalonium	0.5	Nafcillin	0.1
Cefaperazone	1.0	Oxacillin	0.5
Cefapirim	0.5	Penicillin G	0.1
Cefquinome	5.0	Penicillin V	0.5
Chlorotetracycline	5.0	Ronidazol	0.1
Ciprofloxacin	0.5	Sarafloxacine	0.5
Cloxacillin	0.5	Sulfadiazine	0.1
Danofloxacin	1.0	Sulfadimethoxin	0.1
Dapsone	0.1	Sulfadimidin / Sulfamethazine	0.1
Difloxacin	0.5	Sulfadoxin	0.1
Dimetridazol	5.0	Sulfamerazin	0.1
Doramectin*	500.0	Sulfamethoxazole	0.1
Doxycyclin	0.5	Sulfamethoxypyridazine	0.1
Enrofloxacin	0.5	Sulfathiazole	0.1
Eprinomectin	10.0	Tetracycline	0.1
Erythromycine	0.5	Thiamphenicol	0.5
Flumequine	0.5	Trimethoprim	0.1
Ipronidazol-OH	0.1	Tylosine	1.0



With high resolution (70,000 @ *m/z* 200) even trace amounts of target compounds can be detected in matrix.

Targeted screening

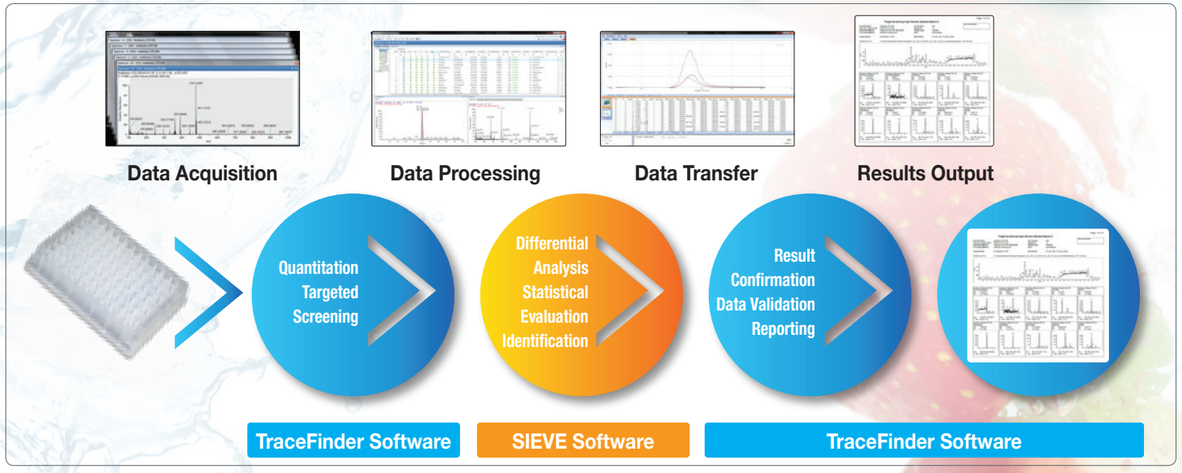
With variable Data Independent Acquisition (vDIA) , the Q Exactive Focus MS delivers data for highly sensitive and selective quantitation, as well for in-depth screening applications. Built-in databases enable quantitation and target screening from a single data set and offer the possibility of retrospective analysis as your database grows.



Relative quantitation for components identified in the unknown screening workflow monitoring degradation in waste water.

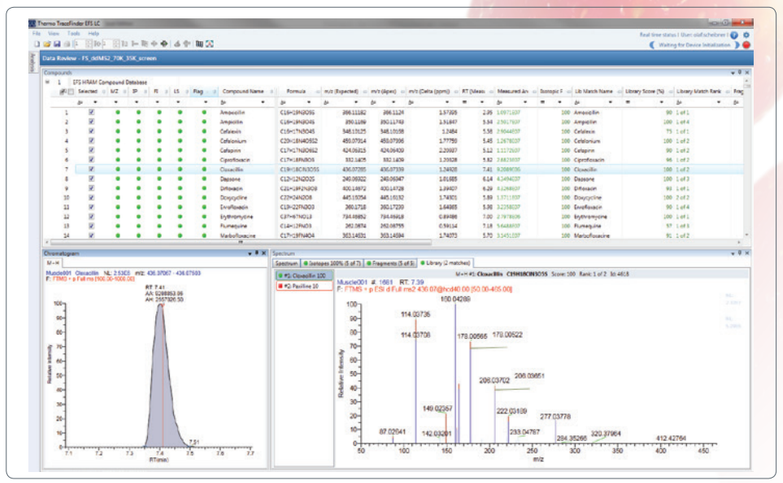
Unknown screening workflow

In addition to targeted screening with vDIA, unknown screening workflows can now be performed using Thermo Scientific™ SIEVE™ software for differential sample analysis (or relative quantitation). Seamlessly integrated into the TraceFinder workflow, SIEVE software performs feature/compound extraction of spectra, followed by differential and statistical analysis to determine compounds that vary significantly within a sample set. The differentially expressed compounds can then be identified using the standard library searching capabilities of TraceFinder software.



High integrated unknown screening workflow with TraceFinder and SIEVE software.

TraceFinder software uses key attributes of HRAM Orbitrap data (to confidently identify compounds accurate mass, isotope abundances, and MS/MS spectral information). TraceFinder HRAM libraries currently include 1,700 food/environmental analyses compounds (including 8,900 HRAM spectra) and 800 clinical research and forensic/toxicological compounds (with 4000 HRAM spectra).



Example of cloxacillin, matching with 100% in muscle matrix at a level of 15ppb.

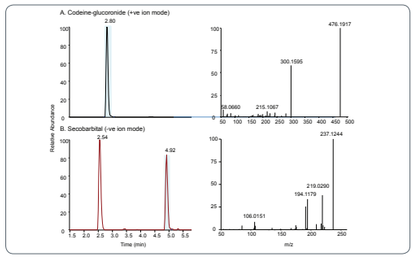
Forensic Toxicology

The ultimate platform for screening and confirmation

Forensic toxicology testing requires confident identification of targeted compound lists in a high-throughput manner followed by quantitative confirmation, plus the ability to identify true unknown compounds. Specificity obtained using proven Orbitrap-based high resolution allows for low limits of detection and quantitation in biological matrices even when short chromatography and simple, low-cost sample preparation such as protein precipitation or dilution are used. Combined with Thermo Scientific™ ToxFinder™ and TraceFinder™ software, the Q Exactive Focus MS offers a powerful, yet simple to use, solution for routine analysis laboratories.

From Screening

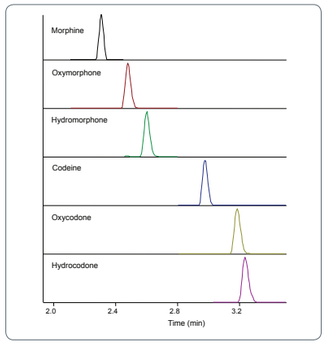
Fast screening with full scan HRAM and data dependent MS^2 ($ddMS^2$) with polarity switching reveal codeine-glucoronide and secobarbital in non-hydrolyzed urine.



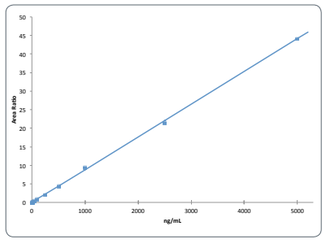
Confirmation of codeine-glucoronide based on accruate *m/z*, retention time, and MS^2 spectrum and isotope pattern matching from HRAM MS and MS/MS data using ToxFinder software.

To Quantitation

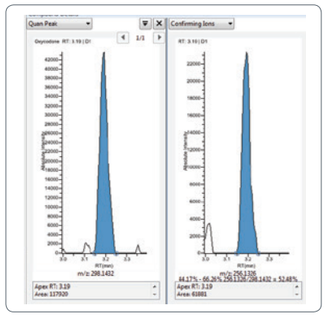
Compounds positively identified/confirmed in screening applications are then quantified, using Parallel Reaction Monitoring (PRM). MS^2 data is collected for both analytes and internal standards. The high resolution of the Q Exactive Focus MS/MS spectra has the benefit of reducing signal contribution from interfering ion species enabling lower levels of quantitation.



Chromatograms extracted from MS^2 spectra obtained from a confirmation PRM experiment for 6 opiates at 5 ng/mL in urine using dilute and shoot method in hydrolyzed and diluted urine.



Representative calibration curve (2.5-5000 ng/mL) from PRM data for oxycodone, demonstrating wide dynamic range and low LOQ to meet sensitivity requirements for demanding assays.



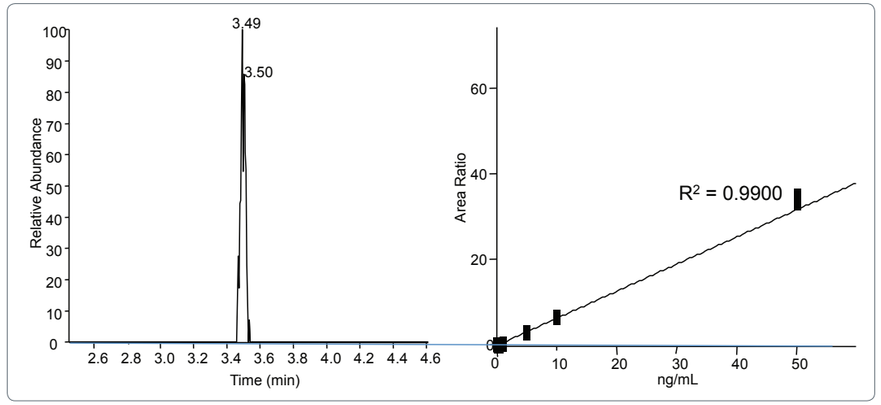
Extracted ion chromatograms for oxycodone at 4.38 ng/mL in donor sample obtained in confirmation PRM experiment .

Pharma and BioPharma Quantitation

Enabling assays from research to routine

The Q Exactive Focus MS has the sensitivity, selectivity and flexibility to provide accurate results for even the most complex bioanalytical assay. The proven Q Exactive platform and ion source robustness assure that validated assays can be performed reliably. Multiple scan functions designed for high performance quantitation can be readily customized to provide optimal performance and tailored to meet the needs of any bioanlaytical assay. The Q Exactive Focus MS provides triple quadrupole-equivalent sensitivity coupled with a resolution setting of 70,000 and 1 ppm mass accuracy, delivering an unprecedented level of selectivity for the accurate quantitation of pharmaceutical compounds in complex matrices.

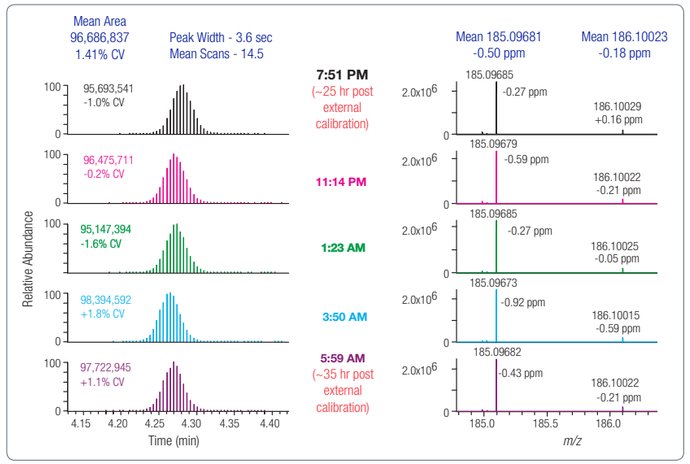
Extracted ion chromatogram for paroxetine at LOQ of 10pgmL in crashed rat plasma matrix.



Calibration curve (10pg/mL – 50 ng/mL) of paroxetine in crashed rat plasma matrix, n=6.

Metabolomics

The Q Exactive Focus MS offers superior and more reliable HRAM performance than Q-TOF instruments. This system provides high scan speed to keep up with UHPLC peak widths, and fast polarity switching to analyze a wide diversity of metabolite compounds in a single analysis.

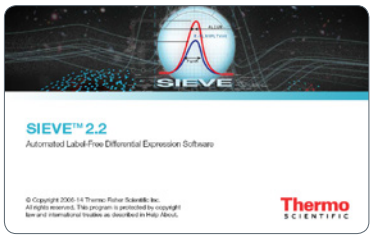


A 12-hour continuous UHPLC-MS analysis of d5 hippuric acid (m/z 185.0969) from rat plasma demonstrates the Q Exactive Focus mass spectrometer's robust ion statistics and highly stable mass accuracy.

Turning Data into Answers

TraceFinder Software

Thermo Scientific TraceFinder 3.2 software is an easy-to-use, workflow-driven software for laboratories performing quantitation and targeted screening using GC-MS and LC-MS. TraceFinder software increases productivity with powerful method development, simplified data acquisition, comprehensive data review, and extensive reporting features including custom report options.

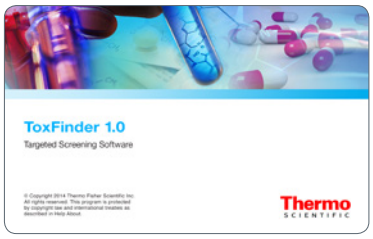


SIEVE Software

Thermo Scientific SIEVE 2.2 software automates differential analysis of metabolites, proteins, and peptides. SIEVE software includes a new advanced algorithm for small molecule peak detection that facilitates large-scale data reduction, reduces false positives, generates elemental composition information, and displays pathway mapping for metabolomics.

Compound Discoverer Software

Thermo Scientific™ Compound Discoverer™ 1.0 software improves how data is stored, processed and reported for small molecule identification. Flexible, user defined workflows enable confident detection and identification for diverse applications such as pharmaceutical MetID, forensic toxicology, environmental research and impurity analysis.



ToxFinder ID Software

Thermo Scientific ToxFinder 1.0 software is a simple, intuitive software application supporting experiment specific workflows from screening to routine semi quantitation. ToxFinder software expedites the method development process with easy to set up databases, experiment based method templates, and advanced algorithms for finding, confirming and quantitating compounds of interest.

Applications:

AN 610: Metabolomic Profiling in Drug Discovery: Understanding the Factors that Influence a Metabolomics Study and Strategies to Reduce Biochemical and Chemical Noise (AN64272-EN)
AN 613: Detection of Stanozolol Glucuronides in Human Sports Drug Testing by Means of High-Resolution, Accurate-Mass Mass Spectrometry (AN64248-EN)
AN 614: Quick and Sensitive Analysis of Multiclass Veterinary Drug Residues in Meat, Plasma, and Milk on a Q Exactive Focus LC-MS System (AN64249-EN)
AN 615: Quantitation of Opiates to Low ng/mL Levels in Urine for Forensic Use Using an Affordable, High-Resolution, Accurate-Mass Mass Spectrometer (AN64257-EN)
AN 617: Quick and Sensitive Analysis of Pesticides Using a Full-Scan Data-Dependent MS/MS Approach on a Q Exactive Focus LC-MS system (AN642824-EN)

Product Specifications:

Q Exactive Focus Product Specification Sheet (PS64233-EN)

For Research Use Only. Not for use in diagnostic procedures.

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